Ligand-breeding procedure

Overlay ligands or macromolecule: ligand complexes

Identify matching bonds in ligands

Remove matching bonds in ligands

Recombine ligand fragments

Save new ligand

Duplicate ligand?

Nes procedure

Overlay ligands or macromolecule: ligands or macromolecule: ligands

yes

Duplicate ligand?

FIG.

 r_1

Dark circles represent atoms, thick lines represent bonds. Thin lines show r₁ and r₂, the distances between the atoms at each end of the bond. The dashed line shows the right-hand bond translated left so that the angle between the two bonds, θ, can be calculated.

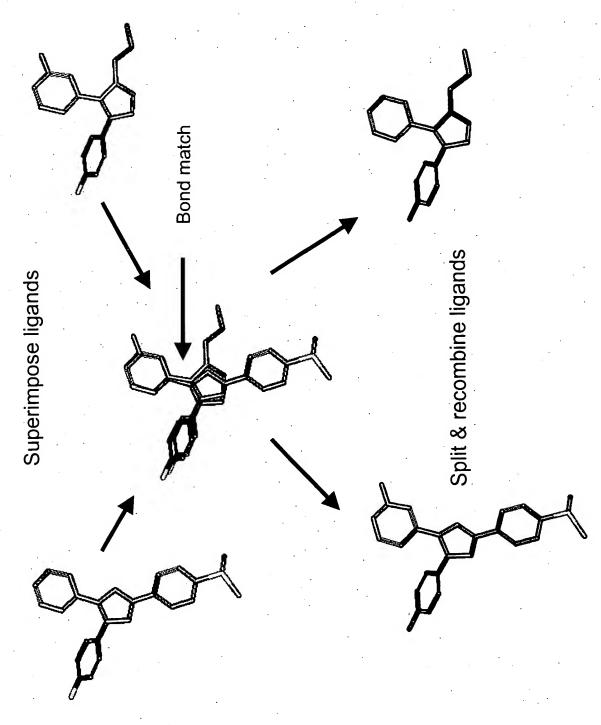


FIG.

